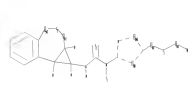
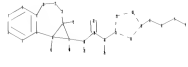
```
     FILE 'REGISTRY' ENTERED AT 11:34:03 ON 26 MAR 2008
L1                STRUCTURE UPLOADED
L2                STRUCTURE UPLOADED
L3             0 S L2
L4                STRUCTURE UPLOADED
L5             0 S L4
L6                STRUCTURE UPLOADED
L7             0 S L6
L8             0 S L6 SSS FULL
L9                STRUCTURE UPLOADED
L10            1 S L9
L11            8 S L9 SSS FULL

     FILE 'CAPLUS' ENTERED AT 11:46:02 ON 26 MAR 2008
L12            5 S L11

     FILE 'HCAPLUS' ENTERED AT 11:47:35 ON 26 MAR 2008
L13        36385 S REVERSE TRANSCRIPTASE
L14         1852 S NON-NUCLEOSIDE
L15       257556 S UREA OR THIOUREA
L16        13764 S CYCLOPROPYL
L17           72 S L13 AND L14 AND L15
L18            3 S L13 AND L14 AND L15 AND L16
L19           45 S L17 AND (PY<2003 OR AY<2003 OR PRY<2003)
L20            3 S L18 AND (PY<2003 OR AY<2003 OR PRY<2003)
```

```
=> file registry
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 11:34:03 ON 26 MAR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   25 MAR 2008  HIGHEST RN 1010115-69-1
DICTIONARY FILE UPDATES:  25 MAR 2008  HIGHEST RN 1010115-69-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10526598structure.str
```





chain nodes :
18 19 20 22 23 25 31 33 34 35 40 41 42
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 26 27 28 29 30
chain bonds :
7-42 8-41 9-18 9-40 18-19 18-23 19-20 19-22 20-25 20-26 29-33 31-33
31-34
34-35
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-10 6-8 7-9 7-8 7-12 8-9 10-11 11-12 26-27
26-30 27-28 28-29 29-30
exact/norm bonds :
5-6 5-10 6-8 7-9 7-8 7-12 7-42 8-9 8-41 9-18 9-40 10-11 11-12 18-19
18-23 19-20 19-22 20-25 20-26 26-27 26-30 27-28 28-29 29-30 29-33 31-33
31-34 34-35

normalized bonds :
1-2 1-6 2-3 3-4 4-5

G1:C,O,S,N

G2:O,S

G3:H,CH3,Et,n-Pr,i-Pr

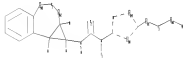
Match level :

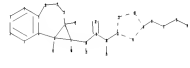
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 18:CLASS 19:CLASS 20:CLASS 22:CLASS 23:CLASS 25:CLASS
26:Atom 27:Atom 28:Atom
29:Atom 30:Atom 31:Atom 33:CLASS 34:CLASS 35:Atom 40:CLASS 41:CLASS
42:CLASS
Generic attributes :
35:
Type of Ring System   : Monocyclic

L1   STRUCTURE UPLOADED

=> s l1
STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large. You may delete
attributes or atoms to reduce the size of the structure
and try again.

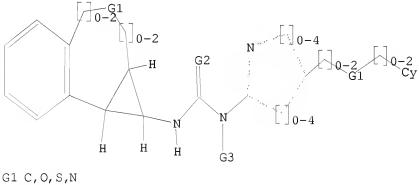
=>
Uploading C:\Program Files\Stnexp\Queries\10526598str2.str





chain nodes :
18 19 20 22 23 25 31 33 34 35 40 41 42
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 26 27 28 29 30

```
chain bonds :
7-42  8-41  9-18  9-40  18-19  18-23  19-20  19-22  20-25  20-26  29-33  31-33
31-34
34-35
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-10  6-8  7-9  7-8  7-12  8-9  10-11  11-12  26-27
26-30  27-28  28-29  29-30
exact/norm bonds :
5-6  5-10  6-8  7-9  7-8  7-12  7-42  8-9  8-41  9-18  9-40  10-11  11-12  18-19
18-23  19-20  19-22  20-25  20-26  26-27  26-30  27-28  28-29  29-30  29-33  31-33
31-34  34-35

normalized bonds :
1-2  1-6  2-3  3-4  4-5


G1:C,O,S,N

G2:O,S

G3:H,CH3,Et,n-Pr,i-Pr

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  18:CLASS  19:CLASS  20:CLASS  22:CLASS  23:CLASS  25:CLASS
26:Atom  27:Atom  28:Atom
29:Atom  30:Atom  31:Atom  33:CLASS  34:CLASS  35:Atom  40:CLASS  41:CLASS
42:CLASS
Generic attributes :
35:
Type of Ring System    : Monocyclic




L2      STRUCTURE UPLOADED

=> d l2
L2 HAS NO ANSWERS
L2                STR
```




```
G1 C,O,S,N
G2 O,S
G3 H,Me,Et,n-Pr,i-Pr
```

Structure attributes must be viewed using STN Express query preparation.

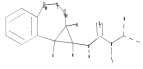
=> s l2
SAMPLE SEARCH INITIATED 11:35:28 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 223 TO ITERATE

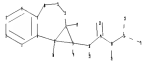
100.0% PROCESSED 223 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3565 TO 5355
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L2

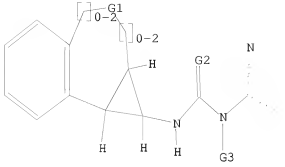
=>
Uploading C:\Program Files\Stnexp\Queries\10526598str3.str





chain nodes :
18 19 20 22 23 25 26 27 28 29 30 31
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12

```
chain bonds :
7-31  8-30  9-18  9-29  18-19  18-23  19-20  19-22  20-25  20-26  26-27  26-28
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-10  6-8  7-9  7-8  7-12  8-9  10-11  11-12
exact/norm bonds :
5-6  5-10  6-8  7-9  7-8  7-12  7-31  8-9  8-30  9-18  9-29  10-11  11-12  18-19
18-23  19-20  19-22  20-25  20-26  26-27  26-28
normalized bonds :
1-2  1-6  2-3  3-4  4-5


G1:C,O,S,N

G2:O,S

G3:H,CH3,Et,n-Pr,i-Pr

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  18:CLASS  19:CLASS  20:CLASS  22:CLASS  23:CLASS  25:CLASS
26:Atom  27:Atom  28:Atom
29:CLASS  30:CLASS  31:CLASS



L4      STRUCTURE UPLOADED

=> s l4
SAMPLE SEARCH INITIATED 11:36:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       15 TO ITERATE

100.0% PROCESSED       15 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           68 TO      532
PROJECTED ANSWERS:               0 TO        0

L5            0 SEA SSS SAM L4

=> d l4
L4 HAS NO ANSWERS
L4              STR
```



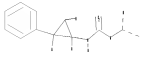
G1 C,O,S,N

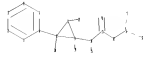
G2 O,S

G3 H,Me,Et,n-Pr,i-Pr

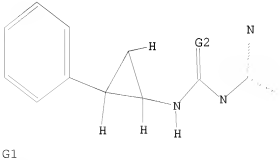
Structure attributes must be viewed using STN Express query preparation.

=>
Uploading C:\Program Files\Stnexp\Queries\10526598str4.str





```
chain nodes :
10  11  12  14  15  16  17  18  19  20  21
ring nodes :
1  2  3  4  5  6  7  8  9
chain bonds :
6-8  7-21  8-20  9-10  9-19  10-11  10-15  11-12  11-14  12-16  16-17  16-18
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-9  7-8  8-9
exact/norm bonds :
7-9  7-8  8-9  9-10  10-11  11-12  11-14  12-16  16-17  16-18
exact bonds :
6-8  7-21  8-20  9-19  10-15
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6


G2:O,S

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  14:CLASS  15:CLASS  16:Atom  17:Atom  18:Atom  19:CLASS
20:CLASS  21:CLASS



L6      STRUCTURE UPLOADED

=> s l6
SAMPLE SEARCH INITIATED 11:37:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        1 TO ITERATE

100.0% PROCESSED        1 ITERATIONS                                 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:             1 TO       80
PROJECTED ANSWERS:                0 TO        0

L7            0 SEA SSS SAM L6

=> d l7
L7 HAS NO ANSWERS
L6              STR
```




```
G1
G2 O,S
```

```
Structure attributes must be viewed using STN Express query preparation.
L7            0 SEA FILE=REGISTRY SSS SAM L6


=> s l6 sss full
FULL SEARCH INITIATED 11:38:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -        5 TO ITERATE

100.0% PROCESSED        5 ITERATIONS                                 0 ANSWERS
SEARCH TIME: 00.00.01

L8            0 SEA SSS FUL L6

=> d his

     (FILE 'HOME' ENTERED AT 11:33:51 ON 26 MAR 2008)

     FILE 'REGISTRY' ENTERED AT 11:34:03 ON 26 MAR 2008
L1              STRUCTURE UPLOADED
L2              STRUCTURE UPLOADED
L3            0 S L2
L4              STRUCTURE UPLOADED
L5            0 S L4
L6              STRUCTURE UPLOADED
L7            0 S L6
L8            0 S L6 SSS FULL

=> log hold
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   181.12     181.33

 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 11:38:21 ON 26 MAR 2008

Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:SSPTAEXO1623

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 11:44:58 ON 26 MAR 2008
FILE 'REGISTRY' ENTERED AT 11:44:58 ON 26 MAR 2008
COPYRIGHT (C) 2008 American Chemical Society (ACS)

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   181.12     181.33

=>
Uploading C:\Program Files\Stnexp\Queries\10526598str5.str
```

chain nodes :
1 5 6 7 9 10 11 12 13 14
ring nodes :
2 3 4
chain bonds :
1-3 2-13 2-14 3-12 4-5 4-11 5-6 5-10 6-7 6-9
ring bonds :
2-4 2-3 3-4
exact/norm bonds :
2-4 2-3 3-4 4-5 5-6 6-7 6-9
exact bonds :
1-3 2-13 2-14 3-12 4-11 5-10

G2:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:CLASS 7:CLASS 9:CLASS 10:CLASS
11:CLASS

12:CLASS 13:CLASS 14:CLASS

L9   STRUCTURE UPLOADED

=> s l9
SAMPLE SEARCH INITIATED 11:45:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   680 TO ITERATE

100.0% PROCESSED   680 ITERATIONS   1 ANSWERS
SEARCH TIME: 00.00.01

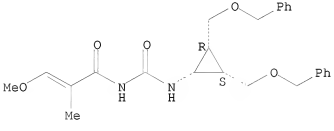
FULL FILE PROJECTIONS: ONLINE   **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 12036 TO   15164
PROJECTED ANSWERS: 1 TO   80

L10   1 SEA SSS SAM L9

=> d l10 scan

L10 1 ANSWERS   REGISTRY COPYRIGHT 2008 ACS on STN
IN   2-Propenamide, N-[[[(1α,2α,3α)-2,3-
     bis[(phenylmethoxy)methyl]cyclopropyl]amino]carbonyl]-3-methoxy-2-methyl-
     (9CI)
MF   C25 H30 N2 O5

Relative stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l9 sss full
FULL SEARCH INITIATED 11:45:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   12485 TO ITERATE

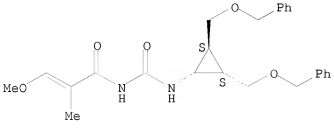
100.0% PROCESSED   12485 ITERATIONS   8 ANSWERS
SEARCH TIME: 00.00.01

L11   8 SEA SSS FUL L9

=> d l11 scan

L11 8 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN   2-Propenamide, N-[[[2,3-bis[(phenylmethoxy)methyl]cyclopropyl]amino]carbon
     yl]-3-methoxy-2-methyl-, (1α,2α,3β)- (9CI)
MF   C25 H30 N2 O5

Relative stereochemistry.
Double bond geometry unknown.

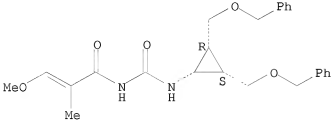


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):7

L11 8 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN   2-Propenamide, N-[[[(1α,2α,3α)-2,3-
     bis[(phenylmethoxy)methyl]cyclopropyl]amino]carbonyl]-3-methoxy-2-methyl-
     (9CI)
MF   C25 H30 N2 O5

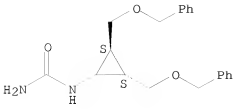
Relative stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 8 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN   Urea, [2,3-bis[(phenylmethoxy)methyl]cyclopropyl]-,
     (1α,2α,3β)- (9CI)
MF   C20 H24 N2 O3

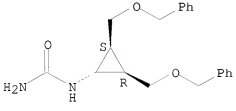
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

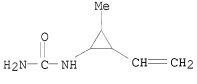
L11 8 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Urea, [2,3-bis[(phenylmethoxy)methyl]cyclopropyl]-, (1α,2β,3β)- (9CI)
MF C20 H24 N2 O3

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

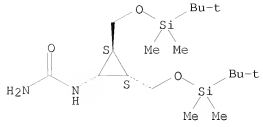
L11 8 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Urea, (2-ethenyl-3-methylcyclopropyl)- (9CI)
MF C7 H12 N2 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 8 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Urea, [2,3-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]cyclopropyl]-, (1α,2α,3β)- (9CI)
MF C18 H40 N2 O3 Si2

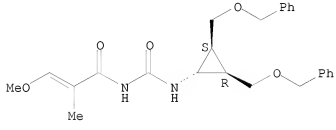
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 8 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Propenamide, N-[[[2,3-bis[(phenylmethoxy)methyl]cyclopropyl]amino]carbonyl]-3-methoxy-2-methyl-, (1α,2β,3β)- (9CI)
MF C25 H30 N2 O5

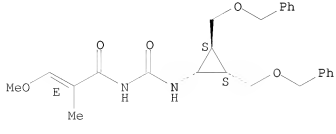
Relative stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 8 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Propenamide, N-[[[2,3-bis[(phenylmethoxy)methyl]cyclopropyl]amino]carbonyl]-3-methoxy-2-methyl-, [1α(E),2α,3β]- (9CI)
MF C25 H30 N2 O5

Relative stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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FULL ESTIMATED COST 359.94 360.15

FILE 'CAPLUS' ENTERED AT 11:46:02 ON 26 MAR 2008
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FILE COVERS 1907 - 26 Mar 2008 VOL 148 ISS 13
FILE LAST UPDATED: 25 Mar 2008 (20080325/ED)

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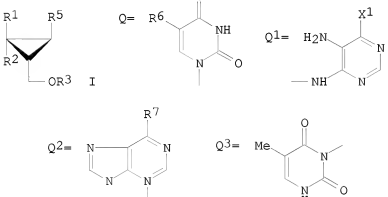
=> s l11
L12 5 L11

=> d l12 1-5 ti abs bib

L12 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
TI Novel preparation of cis,cis-trisubstituted cyclopropane nucleosides
AB Novel cyclopropane nucleosides, cis-2',cis-3'-bis(hydroxymethyl)cyclopropyl thymine and adenine were synthesized. The stereoselective ring contraction of cyclobutyl bromohydrin afforded a cyclopropyl aldehyde with a cis,cis configuration. After oxidation, conversion to amide and Hofmann's rearrangement, the Me carbamate was obtained. Its basic hydrolysis yielded an amine, then the target mols. were obtained by construction of bases.
AN 1999:100564 CAPLUS <<LOGINID::20080326>>
DN 130:196913
TI Novel preparation of cis,cis-trisubstituted cyclopropane nucleosides
AU Gauvry, Noelle; Huet, Francois

CS Laboratoire de Synthese Organique, UPRES A CNRS 6011, Faculte des Sciences, Universite di Maine, Le Mans, F-72085, Fr.
SO Tetrahedron (1999), 55(5), 1321-1328
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of cyclopropane ring-containing nucleic acid bases as antiviral, antitumor, and antibacterial agents
GI



AB Cyclopropane carbocyclic nucleosides (I; 1 of R1, R2 = H, the other = CH2OR4; R3, R4 = H, phenylalkyl; R5 = Q-Q3; R6 = alkyl; X1 = halo; R7 = halo, amino) are prepared as antiviral, antitumor, and antibacterial agents (no data). Thus, heating a solution of 272 mg I (R1 = PhCH2OCH2, R2 = H, R3 = CH2Ph, R5 = NHCONHCOCMe:CHOMe) and NH3 in MeOH at 85° in a sealed tube for 23 h gave 163 mg I (R1 = PhCH2OCH2, R2 = H, R3 = CH2Ph, R5 = Q, R6 = Me) (II) and 37 mg I (R1 = PhCH2OCH2, R2 = H, R3 = CH2Ph, R5 = Q3). Treatment of 340 mg II with BF3 in CH2Cl2 at -78° to room temperature gave 154 mg I (R1 = HOCH2, R2 = H, R3 = H, R5 = Q, R6 = Me).
AN 1992:470271 CAPLUS <<LOGINID::20080326>>
DN 117:70271
TI Preparation of cyclopropane ring-containing nucleic acid bases as antiviral, antitumor, and antibacterial agents
IN Kaneko, Shuetsu; Katagiri, Shinya
PA Otsuka Seiyaku K. K., Japan
SO Jpn. Kokai Tokkyo Koho, 17 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 04074169	A	19920309	JP 1990-188647	19900716
PRAI	JP 1990-188647		19900716		
OS	MARPAT 117:70271				

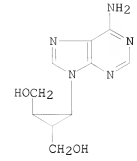
L12 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of cyclopropyl nucleoside analogs with antiviral activity
GI

AB Title compds. [I; A = purin-9-yl, pyrimidin-1-yl, or their isosteres; G,D = H, (un)substituted C1-10 alkyl, OH, CHO, CO2R1, OCH2PO3H2; R1 = H, C1-10 alkyl; provided that one of D or G is other than H or C1-10 alkyl] are prepared Thus, a mixture of 2-(1,2-dihydroxyethyl)cyclopropylamine (preparation given), 2-amino-4,6-dichlorpyrimidine, Et3N, and n-BuOH was refluxed 4 h with stirring to give 47% 1-[(2-amino-6-chloropyrimidin-4-yl)amino]-2-(1,2-dihydroxyethyl)cyclopropane. This was coupled with p-chlorobenzenediazonium chloride in aqueous NaOAc-AcOH buffer to give 65% a diazo compound which was reduced with Zn/AcOH at 70° to give 1-[(2,5-diamino-6-chlorpyrimidin-4-yl)amino]-2-(1,2-dihydroxyethyl)cyclopropane. The latter was stirred 72 h at room temperature with HC(OEt)3 in DMF containing concentrated H2SO4 and the resulting 6-chloropurine derivative was hydrolyzed with 2 N aqueous HCl under reflux to give 9-[2-(1,2-dihydroxyethyl)cyclopropyl]guanine (II). II in vitro showed a virus rating of 1.8 and at 101 μg/mL gave 50% inhibition of virus-induced cytopathogenic effects in E-377 cells challenged with herpes simplex virus.
AN 1991:450218 CAPLUS <<LOGINID::20080326>>
DN 115:50218
TI Preparation of cyclopropyl nucleoside analogs with antiviral activity
IN Norbeck, Daniel W.; Rosen, Terry J.; Sham, Hing L.
PA Abbott Laboratories, USA
SO U.S., 22 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4988703	A	19910129	US 1989-355594	19890522
PRAI US 1989-355594		19890522		

OS MARPAT 115:50218

L12 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
TI Synthesis of nucleosides and related compounds. Part 20. Synthesis of 9-(t-2,c-3-dihydroxymethyl-r-1-cyclopropyl)-9H-adenine (a lower methylene homolog of carbocyclic oxetanocin) and related compounds
GI



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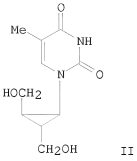

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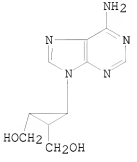

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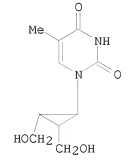

IV

AB To clarify the relationship of side chain conformation and flexibility to biol. activity, a series of carbocyclic analogs of oxetanocin having a one-methylene unit shorter in the cyclobutane ring, 9-(t-2,c-3-dihydroxymethyl-r-1-cyclopropyl)-9H-adenine (I) and the related compds. II-IV were synthesized.
AN 1991:122948 CAPLUS <<LOGINID::20080326>>
DN 114:122948
TI Synthesis of nucleosides and related compounds. Part 20. Synthesis of 9-(t-2,c-3-dihydroxymethyl-r-1-cyclopropyl)-9H-adenine (a lower methylene homolog of carbocyclic oxetanocin) and related compounds
AU Katagiri, Nobuya; Sato, Hiroshi; Kaneko, Chikara
CS Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SO Chemical & Pharmaceutical Bulletin (1990), 38(11), 3184-6
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English

L12 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
TI The diazo route to 2-vinylcyclopropylidenes
GI

I

AB Propylidenes I (R = H, Me; R1 = vinyl, CH:CD2, CH:CHMe) were generated via N2CHCO2Et addition to alkadienes or α,β-unsatd. aldehydes. Wittig reaction of the aldehyde moiety yielded substituted

cyclopropanecarboxylates. Hydrolysis, Curtius degradation, and nitrosation produced due nitrosoureas, which formed I upon addition of base. In MeOH and NaHCO3 I yielded the ring-opened methoxypentadienes. In MeOH-NaOMe the carbene generated from I underwent allene formation and Skattebol rearrangement (L. Skattebol, 1962) competitively. Methoxycyclopentenes occurred in excess over cyclopentadienes. In the presence of CH2:CHOMe, I ring expanded to the cyclopentene carbene, which cycloadded to generate the spiro compds. or underwent electrophilic addition

AN 1986:68476 CAPLUS <<LOGINID::20080326>>
DN 104:68476
OREF 104:10949a,10952a
TI The diazo route to 2-vinylcyclopropylidenes
AU Kirmse, Wolfgang; Van Chiem, Pham; Henning, Paul Georg
CS Abt. Chem., Ruhr-Univ., Bochum, 4630, Fed. Rep. Ger.
SO Tetrahedron (1985), 41(8), 1441-51
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
OS CASREACT 104:68476

=> file stnguide

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	15.03	375.18
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.00	-4.00

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=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.12	375.30
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.00

FILE 'HCAPLUS' ENTERED AT 11:47:35 ON 26 MAR 2008
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FILE COVERS 1907 - 26 Mar 2008  VOL 148 ISS 13
FILE LAST UPDATED: 25 Mar 2008  (20080325/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s reverse transcriptase

        242046 REVERSE
         36995 TRANSCRIPTASE
L13      36385 REVERSE TRANSCRIPTASE
                (REVERSE(W)TRANSCRIPTASE)

=> s non-nucleoside

        950092 NON
         49897 NUCLEOSIDE
L14       1852 NON-NUCLEOSIDE
                (NON(W)NUCLEOSIDE)

=> s urea or thiourea

        223626 UREA
         44764 THIOUREA
L15     257556 UREA OR THIOUREA

=> s cyclopropyl

L16      13764 CYCLOPROPYL

=> s l13 and l14 and l15

L17         72 L13 AND L14 AND L15

=> s l13 and l14 and l15 and l16

L18          3 L13 AND L14 AND L15 AND L16

=> s l17 and (PY<2003 or AY<2003 or PRY<2003)

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       4479974 AY<2003
       3955297 PRY<2003
L19         45 L17 AND (PY<2003 OR AY<2003 OR PRY<2003)

=> s l18 and (PY<2003 or AY<2003 or PRY<2003)

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       4479974 AY<2003
       3955297 PRY<2003
L20          3 L18 AND (PY<2003 OR AY<2003 OR PRY<2003)

=> file stnguide

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 21, 2008 (20080321/UP).

=> d l20 1-3 ti abs bib
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L20 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of amino acid-containing non-nucleoside reverse transcriptase inhibitors
AB Non-nucleoside reverse transcriptase inhibitors Rx-L*-O-Ar1-CHR4CHR5NHC(:Z)NH-Ar2 [Ar1 is an unsatd., optionally substituted, mono- or bicyclic ring structure comprising 0-3 hetero atoms selected from S, O and N; Ar2 is an aromatic, optionally substituted, monocyclic ring structure comprising at least one nitrogen hetero atom and 0-2 further hetero atoms selected from S, O and N; R4, R5 = H, (cyclo)alkyl, alkenyl, alkynyl, alkoxy, alkanoyloxy, alkylthio, amino, carboxy, carbamoyl, cyano, halo, hydroxy, aminomethyl, hydroxymethyl, carboxymethyl, haloalkylthio, nitro; or R4 and R5 join to form a 3-6 membered, optionally substituted ring structure; Z = O or S; Rx is the residue of a natural or unnatural amino acid; L* is a linker moiety which is ether, carbonate or ester] or their pharmaceutically-acceptable salts were prepared as anti-HIV agents with favorable pharmacokinetic properties. Thus, (1S,2S)-N-[cis-2-(6-fluoro-2-(L-valyloxy)methoxycarbonyloxy-3-propionylphenyl)cyclopropyl]-N'-[2-(5-cyanopyridyl)]urea was prepared and showed 70% bioavailability of released drug at a dose of 0.027 mmol/kg after 6 h in a rat bioavailability assay model.
AN 2002:696666 HCAPLUS <<LOGINID::20080326>>
DN 137:217244
TI Preparation of amino acid-containing non-nucleoside reverse transcriptase inhibitors
IN Zhou, Xiao-xiong; Johansson, Nils-Gunnar; Wahling, Horst; Sund, Christian; Salvador, Lourdes; Lindstrom, Stefan; Wallberg, Hans; Sahlberg, Christer
PA Medivir AB, Swed.
SO U.S. Pat. Appl. Publ., 40 pp., Cont.-in-part of Appl. No. PCT/SE99/01403.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002128301	A1	20020912	US 2001-927254	20010810 <--
	ZA 9807267	A	19990215	ZA 1998-7267	19980813 <--
	WO 9909031	A1	19990225	WO 1998-SE1467	19980814 <--

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     NZ 508502           A     20020426    NZ 1998-508502          19980814 <--
     CN 1872869          A     20061206    CN 2006-10099722        19980814 <--
     ZA 9901148          A     19990812    ZA 1999-1148            19990212 <--
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     WO 2000047561       A1    20000817    WO 1999-SE1403          19990818 <--
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PRAI SE 1998-452         A     19980213  <--
     SE 1998-469         A     19980216  <--
     SE 1998-1216        A     19980403  <--
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     SE 1997-2957        A     19970815  <--
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OS   MARPAT 137:217244

L20  ANSWER 2 OF 3  HCAPLUS  COPYRIGHT 2008 ACS on STN
TI   Tricycloalkatrienes as non-nucleoside reverse
     transcriptase inhibitors
GI
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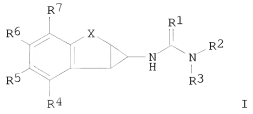

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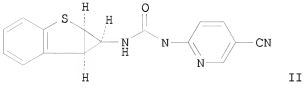

II

AB Title compds. I [R1 = O, S; R2 = (un)substituted nitrogen-containing heterocycle, wherein the nitrogen is located at the 2 position relative to the (thio)urea bond; R3 = H, alkyl; R4-R7 = H, alkyl, alkenyl, alkynyl, haloalkyl, alkanoyl, haloalkanoyl, alkoxy, haloalkoxy, alkyloxyalkyl, haloalkyloxylkyl, hydroxyalkyl, aminoalkyl, carboxyalkyl, cyanoalkyl, amino, carboxy, carbamoyl, cyano, halo, hydroxy, keto; X = (CHR8)nD(CHR8)m; D = NR9, O, S, S(=O), SO2; R8 = H, alkyl, haloalkyl; R9 = H, alkyl; n, m = 0, 1, 2] and prodrugs and pharmaceutically acceptable salts thereof, have utility as inhibitors of HIV-1 reverse transcriptase, particularly drug escape mutants. Thus, benzothiophene was treated with N2CHCO2Et to give Et cis-1a,6b-dihydro-1H-benzo[b]cyclopropa[d]thiophene-1-carboxylate which was hydrolyzed to the acid and treated with (PhO)2PN3 and 2-amino-6-cyanopyridine to give the urea II. II had ED50 in the XTT assay with wild-type HIV-1IIIB of 2 nM.

AN 2002:695980 HCAPLUS <<LOGINID::20080326>>

DN 137:232544

TI Tricycloalkatrienes as non-nucleoside reverse transcriptase inhibitors

IN Lindstroem, Stefan; Sahlberg, Christer; Wallberg, Hans; Kalyanov, Genaidy; Oden, Lourdes; Naeslund, Lotta

PA Medivir AB, Swed.

SO PCT Int. Appl., 106 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002070516	A2	20020912	WO 2002-EP2328	20020304 <--
	WO 2002070516	A3	20030206		

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CN	101081843	A	20071205	CN 2006-10082490	20020304 <--
US	2003069224	A1	20030410	US 2002-92752	20020305 <--
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US	2003187266	A1	20031002	US 2003-377057	20030228 <--
US	6894177	B2	20050517		
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MX	2003PA08040	A	20040524	MX 2003-PA8040	20030905 <--
HK	1063784	A1	20070309	HK 2004-106555	20040831 <--
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TI Colorimetric assays for evaluation of the mode of action of human immunodeficiency virus type 1 non-nucleoside reverse transcriptase inhibitors

AB Four non-nucleoside reverse transcriptase (RT) inhibitors, 9-Cl-TIBO [(+)-S-4,5,6,7-tetrahydro-9-chloro-5-methyl-6-(3-methyl-2-butenyl)imidazo(4,5,1-jk)(1,4)-benzodiazepin-2(1H)-thione], nevirapine (6,11-dihydro-11-cyclopropyl-4-methyl-dipyrido[2,3-b:2',3'-e]-[1,4]diazepin-6-one), MSA-300 (N-[cis-2-(2-hydroxy-3-acetyl-6-methoxy-phenyl)-cyclopropyl]-N'-(5-chloropyrid-2-yl)-thiourea) and delavirdine {1-(5-methanesulfonamido-1H-indol-2-yl-carbonyl)-4-[3-(1-methylethylamino)pyridinyl]piperazine} were analyzed for the mode of action of their inhibition of human immunodeficiency virus type 1 (HIV-1) RT in three different assays utilizing a 96-well microtiter plate format, with solid-phase conjugated poly(rA) as template. These were: (i) direct RT assay, for determination of IC50 values of RT inhibitors; (ii) RT template/primer binding inhibition (BIC) assay, for measuring the effect of various substances on the RT activity binding to template/primer; (iii) RT protein ELISA, for measuring RT protein binding to template/primer with a monoclonal antibody reactive against a peptide in the RNase H region. MSA-300 and delavirdine gave the lowest IC50 values, ranging from 0.17 μM to 0.24 μM for MSA-300 and from 0.12 μM to 0.38 μM for delavirdine, whereas higher IC50 values of approx. 20 μM were obtained for 9-Cl-TIBO at all primer concns. None of the non-nucleoside concns. None of the non-nucleoside substances had inhibiting effects on the binding of template, primer, or template/primer to RT protein. Their inhibition of RT activity was not due to prevention of RT binding to template/primer. TIBO, nevirapine and delavirdine bound to rt reversibly, and they bound more tightly to RT template/primer ternary than to RT template binary complex. MSA-300 showed a comparatively high affinity for the enzyme. The utility of the three assays in relation to screening and anal. of RT inhibitory

substances is discussed.

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